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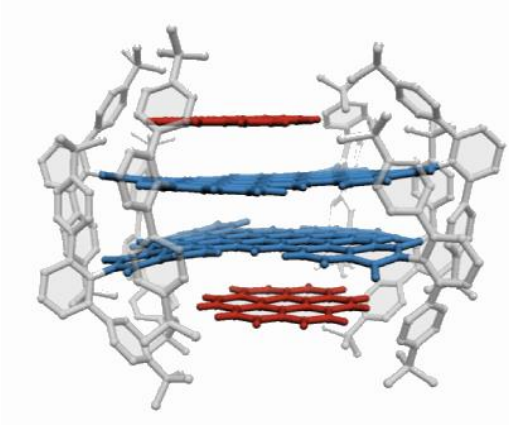
Abstract

Natural photosystems showcase the importance of supramolecular organization for advanced functional properties. Nevertheless, the development of molecular materials is still mostly initiated by purely molecular considerations whilst the influence of intermolecular couplings is only addressed at a later stage.



For a period of more than twenty years our group has explored an alternative approach. Thus, we have studied the formation of molecular aggregates and the functional properties originating from the interaction of π-systems in terms of structure-function relationships. In this lecture I will showcase examples from our most recent research on perylene bisimide (PBI) dyes[1] as well as smaller and larger polycyclic aromatic (multi-)imides for which we could accomplish structurally well-characterized supramolecular aggregate structures[2] and obtain insight into their photofunctional properties. With the advancement of our knowledge, most recently also tailored supramolecular environments are utilized for the engineering of desired functional properties in molecular aggregates which includes (circularly polarized) fluorescence, phosphorescence and thermally activated delayed fluorescence.[3] Finally, a most recent example of supramolecular engineering based on a porous nanographene bilayer will be discussed.[4]

References
[1] R. K. Dubey, F. Würthner, *Nat. Chem.* 2023, *15*, 884: Playing Lego with perylene dyes.
[2] M. Mahl, M. A. Niyas, K. Shoyama, F. Würthner, *Nat. Chem.* 2022, *14*, 457: Multilayer stacks of polycyclic aromatic hydrocarbons.
[3] J. Rühe, K. Vinod, H. Hoh, K. Shoyama, M. Hariharan, F. Würthner, *J. Am. Chem. Soc.* 2024, *146*, 28222: Guest-Mediated Modulation of Photophysical Pathways in a Coronene Bisimide Cyclophane.
[4] M. A. Niyas, K. Shoyama, M. Grüne, F. Würthner, *Nature* 2025, *637*, 854: Bilayer nanographene reveals halide permeation through a benzene hole.

Biosketch

Frank Würthner received his education in Chemistry at the University of Stuttgart (doctoral degree 1994 with Franz Effenberger) and carried out postdoctoral research at MIT in Cambridge/MA (1994/1995 with Julius Rebek, Jr.). After two years at BASF and five years at the University of Ulm (Habilitation in 2001) he became chair professor of Organic Chemistry at the University of Würzburg in 2002. Here he has served as head of the Institute of Organic Chemistry, dean of the Chemistry Department and founding director of the Center for Nanosystems Chemistry.

His main research interests include the synthesis of π-conjugated molecules and functional dyes, their application in organic electronics, photonics and photovoltaics, the construction of complex supramolecular architectures composed of π-scaffolds, the mechanistic elucidation of self-assembly processes, and the investigation of light-induced processes in dye-based nanosystems.

He has published more than 600 papers and is listed since 2014 among the highly cited scientists. He is an elected member of the German National Academy of Science Leopoldina and the Bavarian Academy of Sciences, as well as a Fellow of the Royal Society of Chemistry. His awards include the Arnold-Sommerfeld-Prize of the Bavarian Academy of Science (2002), the Hermanos-Elhuyar-Hans-Goldschmidt Award Lectureship of the Real Sociedad Española de Química (2016), an ERC Advanced Grant (2017), the Ta-shue Chou award of Academia Sinica in Taiwan (2018)), and the Adolf-von-Baeyer Medal of the German Chemical Society (2019).